

## The infrared and Raman investigation of fumaronitrile and maleonitrile

J Marshall

Department of Physics, Loyola College, Chennai-600 034, India.

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**Abstract** The two dicyanoethylenes maleonitrile and fumaronitrile are cis-trans isomers with molecular formula  $(\text{CN})_2\text{C}_2\text{H}_2$ . Fumaronitrile belongs to  $\text{C}_{2h}$  point group while Maleonitrile belongs to  $\text{C}_{2v}$  point group of symmetry of the molecule. The Raman Spectra was obtained on a neat solid in the range  $3400\text{--}50\text{ cm}^{-1}$  and the infrared spectra in the range  $3800\text{--}400\text{ cm}^{-1}$  was examined as fluorolube and Nujol (below  $1350\text{ cm}^{-1}$ ) mulls. The vibrational spectra for the two compounds and their assignments have been reported earlier but they are incomplete, contradictory and questionable in some of the band assignments. Moreover the assignment have not been verified through normal coordinate analysis. In the present paper, a complete assignment is proposed for fumaronitrile and maleonitrile and verified through normal coordinate analysis. Some of the fundamentals in the far-IR have been taken from the earlier work and used for assignment and calculations. The force constants evaluated are in good agreement with constants of similar bonds in other related molecules of the cyanoethylene molecular series.

**Keywords** Infrared and Raman spectra, fumaronitrile and maleonitrile, assignment

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### 1. Introduction

The fumaronitrile and maleonitrile are the two dicyanoethylenes which have been the least studied. The various cyanoethylenes that have been investigated in particular the parent compound acrylonitrile [1-2], malononitrile [3], dicyanoethylenes [4-7], tricyanoethylenes [5] and tetracyanoethylenes [8, 9]. The maleonitrile and fumaronitrile have the same molecular formula  $(\text{CN})_2\text{C}_2\text{H}_2$  but are the cis and trans isomer of the same compound. Fumaronitrile belongs to  $\text{C}_{2h}$  point group, so the rule of mutual exclusion permits only the frequencies of the gerade modes to appear in the Raman spectrum of the compound. The cis isomer maleonitrile belongs to  $\text{C}_{2v}$  symmetry and except for the Raman active  $\text{A}_2$  species all other modes are infrared and Raman active.

Address for Communication : AP 745, G-Block, Anna Nagar West, Chennai-40, India

## 2. Normal coordinate analysis

### Symmetry coordinates :

A set of symmetry coordinates based on the internal coordinates has been constructed for fumaronitrile. The same set of symmetry coordinates is also used for maleonitrile with the coordinates distributed among the  $A_1$ ,  $B_1$ ,  $A_2$  and  $B_2$  species of the  $C_{2v}$  point group of symmetry of the molecule. A set of symmetry coordinates based on the valence coordinates indicated in Figure 1(a) has been constructed for fumaronitrile. The geometrical configuration and structural parameters for maleonitrile is shown in Figure 1(b).

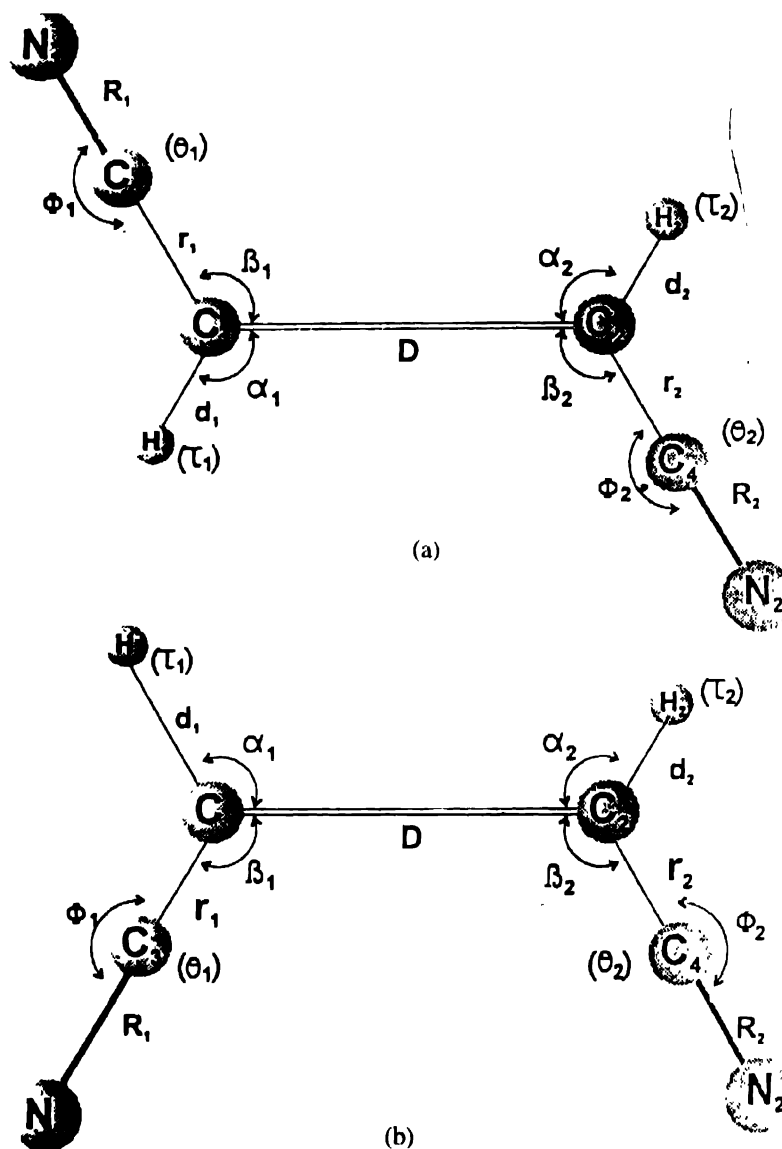


Figure 1. Geometrical configuration and internal coordinates of (a) Fumaronitrile and (b) Maleonitrile.

**Species A<sub>g</sub>**

$$\begin{aligned}
 S_1 &= 1/\sqrt{2}(\Delta d_1 + \Delta d_2) \\
 S_2 &= 1/\sqrt{2}(\Delta R_1 + \Delta R_2) \\
 S_3 &= \Delta D \\
 S_4 &= 1/\sqrt{2}(\Delta \alpha_1 + \Delta \alpha_2) \\
 S_5 &= 1/\sqrt{2}(\Delta r_1 + \Delta r_2) \\
 S_6 &= 1/\sqrt{2}(\Delta \beta_1 + \Delta \beta_2) \\
 S_7 &= 1/\sqrt{2}(\Delta \phi_1 + \Delta \phi_2)
 \end{aligned}$$

**Species B<sub>g</sub>**

$$\begin{aligned}
 S_{11} &= 1/\sqrt{2}(\Delta \tau_1 - \Delta \tau_2) \\
 S_{12} &= 1/\sqrt{2}(\Delta \theta_1 - \Delta \theta_2)
 \end{aligned}$$

**Species A<sub>u</sub>**

$$\begin{aligned}
 S_8 &= 1/\sqrt{2}(\Delta \tau_1 + \Delta \tau_2) \\
 S_9 &= 1/\sqrt{2}(\Delta \theta_1 + \Delta \theta_2) \\
 S_{10} &= S\delta(\text{torsional})
 \end{aligned}$$

**Species B<sub>u</sub>**

$$\begin{aligned}
 S_{13} &= 1/\sqrt{2}(\Delta d_1 - \Delta d_2) \\
 S_{14} &= 1/\sqrt{2}(\Delta R_1 - \Delta R_2) \\
 S_{15} &= 1/\sqrt{2}(\Delta \alpha_1 - \Delta \alpha_2) \\
 S_{16} &= 1/\sqrt{2}(\Delta r_1 - \Delta r_2) \\
 S_{17} &= 1/\sqrt{2}(\Delta \beta_1 - \Delta \beta_2) \\
 S_{18} &= 1/\sqrt{2}(\Delta \phi_1 - \Delta \phi_2)
 \end{aligned}$$

where D, R, d and r represent the appropriate equilibrium distances and stretching coordinates of C=C, C≡N, C-H and C-C bonds respectively;  $\alpha$ ,  $\beta$  and  $\phi$  represent the in-plane bending coordinates,  $\tau$  and  $\theta$  represent the out-of-plane bending coordinate of the respective bond angles. As these molecules have not been studied in detail, the necessary structural parameters have been taken from related cyanoethylenes and used for calculations: (A<sup>0</sup> unit)

$$\begin{aligned}
 D &= 1.363, & \alpha &= \beta = 120^\circ (\text{approx.}) \\
 R &= 1.165, & \phi &= 179^\circ 30' \\
 r &= 1.44, \\
 d &= 1.07.
 \end{aligned}$$

### 3. Results and discussion

#### *The infrared and Raman band assignments for fumaronitrile :*

Fumaronitrile has  $C_{2h}$  symmetry with its eighteen vibrational modes distributed among the species as  $\Gamma_{vib} = 7A_g(R) + 6B_u(IR) + 3A_u(IR) + 2B_g(R)$ . The  $7A_g$  and  $6B_u$  modes correspond to the in-plane vibrations while the  $3A_u$  and  $2B_g$  modes correspond to out-of-plane vibrations of the molecule. The infrared and Raman spectra of fumaronitrile are shown in Figures 2 and 3 respectively. The assignments for fumaronitrile is straightforward as the molecule possesses centre of symmetry. The assignment of C-H, C $\equiv$ N, C=C and C-C stretching modes in the  $A_g$  species are fairly simple and assigned to the frequencies at 3050, 2215, 1610 and 1010  $\text{cm}^{-1}$  respectively. The in-plane bendings are the C=C-H, C=C-C and C-C $\equiv$ N occurring in the Raman spectrum at 1290, 596 and 265  $\text{cm}^{-1}$  respectively. The assignments in the  $A_g$  species agree with the assignments of Long and George (4) and Devlin *et al* [5]. The three stretching fundamentals in the IR active  $B_u$  class are 3070  $\text{cm}^{-1}$  ( $\nu_{13}$ ), 2225  $\text{cm}^{-1}$  ( $\nu_{14}$ ) and 1000  $\text{cm}^{-1}$  ( $\nu_{10}$ ) modes of vibration. The calculated frequency of the  $\nu_{10}$  mode is 1056  $\text{cm}^{-1}$  with 80 percent potential energy distribution (P.E.D.). The assignment of C-H and C=C-C in-plane bendings to 1260  $\text{cm}^{-1}$  and 540  $\text{cm}^{-1}$  in the infrared spectrum agree with the previous workers. The C-C $\equiv$ N bend assigned to 360  $\text{cm}^{-1}$  totally disagrees with the assignment of this mode to about 180  $\text{cm}^{-1}$  by Long and Devlin *et al*. Long [4] has reported having observed a weak IR absorption band at 383  $\text{cm}^{-1}$  in Nujol mull for fumaronitrile. Miller *et al* [9] did not observe this band in the spectrum of solid sample but have inferred a strong absorption at about 360  $\text{cm}^{-1}$  from the combination bands. The assignment of ( $\nu_{18}$ ) mode to 360  $\text{cm}^{-1}$  is supported with a P.E.D of 89 percent from normal coordinate analysis. In carbonyl cyanide Bates *et al* [7] has assigned this mode of vibration to 244  $\text{cm}^{-1}$ . The  $\nu_8$  and  $\nu_9$  modes assigned

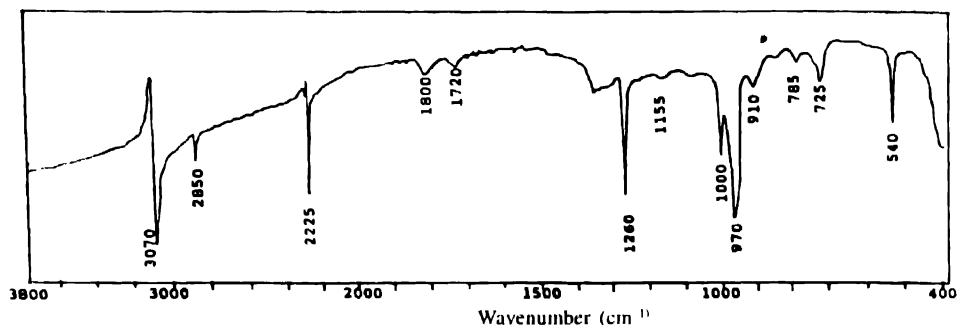


Figure 2. Infrared spectrum of fumaronitrile

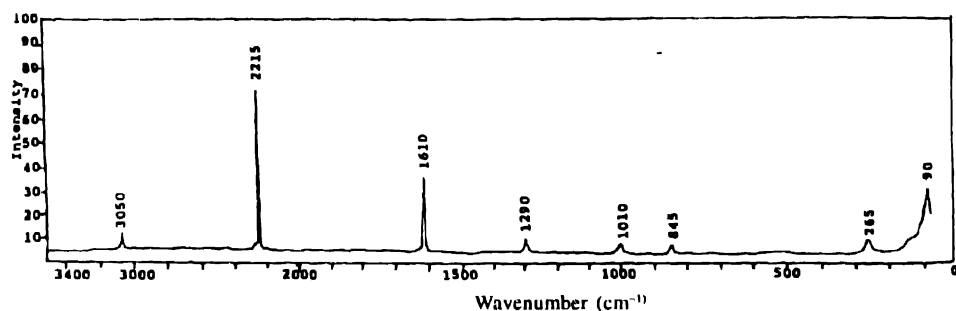


Figure 3. Raman spectrum of fumaronitrile.

to  $785\text{ cm}^{-1}$  and  $150\text{ cm}^{-1}$  are the C-H and C-C≡N out-of-plane vibrations. The torsional mode is too weak to be observed in the far-IR but has been calculated to occur at  $121\text{ cm}^{-1}$ . The two Raman active  $B_g$  fundamentals are at  $845\text{ cm}^{-1}$  ( $\nu_{11}$ ) and  $251\text{ cm}^{-1}$  ( $\nu_{12}$ ). Devlin *et al* [5] have observed a Raman band at about  $250\text{ cm}^{-1}$  and also an overtone of this band in the solution spectrum of fumaronitrile. Long and George [4] report no band in this region of Raman spectrum on solid sample. However in the present investigation a Raman band at  $265\text{ cm}^{-1}$  has been observed and assigned to the ( $\nu_7$ ) mode in  $A_g$  species while the liquid frequency at  $251\text{ cm}^{-1}$  is assigned to the out-of plane ( $\nu_{12}$ ) mode of vibration. The vibrational assignment with P.E.D. is in Table 1.

Table 1. Raman and infrared spectra of fumaronitrile

Frequency ( $\text{cm}^{-1}$ )		Assignment		P.E.D. (%)
Raman	Infrared			
	3070 (VS)	$\nu_{13}$	$\nu_{\text{CH}}$	(99)
3050 (16)		$\nu_1$	$\nu_{\text{CH}}$	(99)
	2850 (M)		$2 \times 785 + 1260$	
2215 (73)		$\nu_2$	$\nu_{\text{C}\equiv\text{N}}$	(99)
	2225 (S)	$\nu_{14}$	$\nu_{\text{C}\equiv\text{N}}$	(100)
	1800 (VW)		$3070 - 1260$	
	1720 (VW)		$2 \times 1260 - 785$	
1610 (37)		$\nu_3$	$\nu_{\text{C}=\text{C}}$	(97)
	1260 (S)	$\nu_{15}$	$\alpha_{\text{CH}}$	(100)
1290 (10)		$\nu_4$	$\alpha_{\text{CH}}$	(92)
	1155 (VW)		$2225 - 2 \times 540$	
	1000 (M)	$\nu_{16}$	$\nu_{\text{CC}}$	(80)
1010 (05)		$\nu_5$	$\nu_{\text{CH}}$	(58)
	970 (VS)		$2225 - 1260$	
	910 (VW)		$2 \times 1000 - 2 \times 540$	
845 (05)		$\nu_{11}$	$A_{g1}$	(100)
	785 (VW)	$\nu_8$	$\nu_{\text{CH}}$	(99)
	725 (VW)		$2 \times 1260 - 785$	
	540 (W)	$\nu_{17}$	$\alpha_{\text{C}=\text{C}-\text{C}}$	(71)
265 (09)		$\nu_7$	$\alpha_{\text{C}-\text{C}\equiv\text{N}}$	(87)
150 (07)		$\nu_9$	$\beta_{\text{C}-\text{C}\equiv\text{N}}$	(97)
90 (30)			Lattice	

$\nu$  - Stretching,  $\alpha$  - In-plane bending,  $\beta$  - Out-of-plane bending. VS-Very Strong, S - Strong, M - Medium, W - Weak, VW - Very Weak  
(number within parentheses are relative intensities)

#### The infrared and Raman band assignments for maleonitrile :

Maleonitrile belongs to  $C_{2v}$  point group of symmetry with its eighteen fundamentals falling under the class  $7A_1$  (R and IR) +  $6B_1$  (R and IR) +  $3A_2$  (R) +  $2B_2$  (R and IR). The thirteen  $A_1$  and

$B_1$  modes correspond to in-plane vibrations while the five  $A_2$  and  $B_2$  modes to the out-of-plane vibrations. The infrared and Raman spectra of maleonitrile are shown in Figures 4 and 5 respectively. In the  $A_1$  species all other modes except the  $\nu_7$  mode are in agreement with Devlin *et al* [9]. He has assigned this mode to a frequency at  $126\text{ cm}^{-1}$  while the same mode has been assigned to a frequency at  $874\text{ cm}^{-1}$  by Long and George (4). Also the  $\nu_7\text{ C}\equiv\text{C}$  mode is placed below the  $\text{C}-\text{C}\equiv\text{N}$  mode in the  $A_1$  species at  $126\text{ cm}^{-1}$  while in  $B_2$  species the corresponding asymmetric vibration is placed at  $714\text{ cm}^{-1}$  very much above the  $\text{C}-\text{C}\equiv\text{N}$  vibration of the species without real conviction. In comparison with fumaronitrile, the deviation of this assignment is too large and without the basis of calculation from normal coordinate analysis. The present assignment with good P.E.D. from calculations places the  $\nu_6$  and  $\nu_7$  mode at  $480\text{ cm}^{-1}$  and  $378\text{ cm}^{-1}$  respectively in the  $A_1$  species. The assignment of  $\text{C}-\text{C}\equiv\text{N}$  i.p. bending to  $378\text{ cm}^{-1}$  is a frequency observed in the IR and Raman spectrum of maleonitrile on liquid sample (9). The corresponding asymmetric  $\nu_{17}$  and  $\nu_{18}$  modes in the  $B_1$  species are at  $595\text{ cm}^{-1}$  and  $463\text{ cm}^{-1}$  respectively. The  $\nu_{18}$  mode assigned to  $463\text{ cm}^{-1}$  has been observed as a weak IR absorption on liquid sample (9). The other assignments of  $B_1$  species at  $3070\text{ cm}^{-1}$  ( $\nu_{13}$ ),  $2240\text{ cm}^{-1}$  ( $\nu_{14}$ ),  $1372\text{ cm}^{-1}$  ( $\nu_{15}$ ) and  $1018\text{ cm}^{-1}$  ( $\nu_{16}$ ) have been found to be correct. The three fundamentals of the Raman active  $A_2$  species are the  $\text{C}-\text{H}$  and  $\text{C}-\text{C}\equiv\text{N}$  o.p. bendings at  $770$  and  $275\text{ cm}^{-1}$  respectively. The torsional mode is assigned to  $112\text{ cm}^{-1}$ . Devlin *et al* have placed the torsional mode too high at  $588\text{ cm}^{-1}$ . A strong band appears in the infrared spectrum at  $770\text{ cm}^{-1}$  which complicates the assignment of the  $\text{C}-\text{H}$  o.p. bend in the  $A_2$  species. This assignment is proved as correct through calculations. Devlin *et al* have not assigned this  $\nu_8$  mode but have assigned the  $770\text{ cm}^{-1}$  band to  $\nu_{11}$  mode in  $B_1$  species. The  $\text{C}-\text{H}$  and  $\text{C}-\text{C}\equiv\text{N}$  o.p. vibrations in the  $B_2$

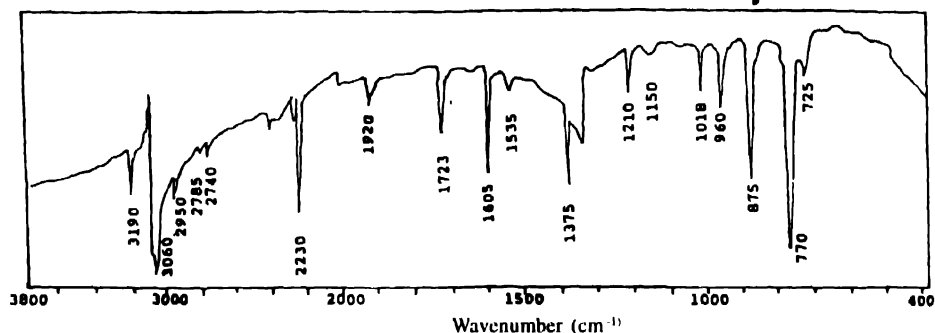


Figure 4. Infrared spectrum of maleonitrile.

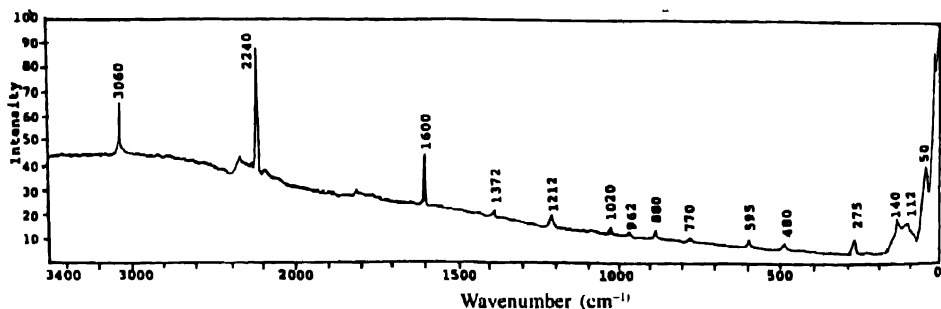


Figure 5. Raman spectrum of maleonitrile.

species have been assigned to  $880\text{ cm}^{-1}$  and  $268\text{ cm}^{-1}$  respectively. The frequency of the  $\nu_{12}$  mode has been substituted from Ref.9. The vibrational assignment with P.E.D. in parentheses for maleonitrile is given in Table 2.

Table 2. Raman and infrared spectra of maleonitrile.

Frequency ( $\text{cm}^{-1}$ )		Assignment	P.E.D. (%)
Raman	Infrared		
	3190 (M)	$2 \times 1605$	
3060 (67)	3060 (VS)	$\nu_1, \nu_{13}$ $\nu_{\text{CH}}$	(99)
	2950 (M)	$1600 + 1375$	
	2785 (M)	$2 \times 960 + 875$	
	2740 (M)	$2 \times 1375$	
2240 (89)	2230 (S)	$\nu_2, \nu_{14}$ $\nu_{\text{C}\equiv\text{N}}$	(99)
	1920 (W)	$2 \times 960$	
	1723 (M)	$2 \times 1375 - 1018$	
1600 (45)	1605 (M)	$\nu_3$ $\nu_{\text{C}=\text{C}}$	(98)
	1535 (W)	$2 \times 770$	
1372 (22)	1375 (S)	$\nu_{15}$ $\alpha_{\text{CH}}$	(100)
1212 (20)	1210 (W)	$\nu_4$ $\alpha_{\text{CH}}$	(92)
	1150 (VW)	$2 \times 1018 - 875$	
1020 (12)	1018 (W)	$\nu_{16}$ $\nu_{\text{CC}}$	(72)
962 (11)	960 (M)	$\nu_5$ $\nu_{\text{CC}}$	(68)
880 (13)	875 (S)	$\nu_{11}$ $\beta_{\text{CH}}$	(100)
770 (10)	770 (VS)	$\nu_8$ $\beta_{\text{CH}}$	(99)
	725 (VW)	$1605 - 875$	
595 (10)		$\nu_{17}$ $\alpha_{\text{C}\equiv\text{C}-\text{C}}$	(70)
480(08)		$\nu_6$ $\alpha_{\text{C}\equiv\text{C}-\text{C}}$	(43)
275(10)		$\nu_9$ $\beta_{\text{C}-\text{C}\equiv\text{N}}$	(91)
140(20)		$2 \times 1600 - 3060$	
112(17)		$\nu_{10}$ $\delta$ (torsion)	(99)
50(40)		Lattice	

$\nu$  - Stretching,  $\alpha$  - In-plane bending,  $\beta$  - Out-of-plane bending VS-Very Strong, S - Strong, M - Medium, W - Weak, VW - Very Weak  
(number within parentheses are relative intensities)

#### Force fields :

The elements of the G-matrix were constructed from the proposed symmetry coordinates and using Wilson's (10)  $S_j^i$  vectors. The secular equation has been evaluated by the kinetic constant method. The kinetic constants are related to the symmetric force constants through the expression

$$\frac{F_{ij}}{F_{jj}} = \frac{K_{ij}}{K_{jj}} \quad (i < j),$$

The assigned vibrational frequencies have been checked for their veracity by calculating the potential energy distribution. The Table 3 gives the observed and calculated frequencies from normal coordinate analysis for fumaronitrile and maleonitrile. The final set of elements of the potential energy matrix adjusted to reproduce accurately the observed frequencies for each species is presented in Table 4 for fumaronitrile and Table 5 for maleonitrile.

**Table 3.** Assignments of fundamentals for fumaronitrile and maleonitrile.

Frequency Mode	Schematic Description	Fumaronitrile (C <sub>2h</sub> )			Maleonitrile (C <sub>2v</sub> )		
		Sym Class	Frequency (cm <sup>-1</sup> )		Sym. Class	Frequency (cm <sup>-1</sup> )	
			Obs.	Cal		Obs.	Cal
$\nu_1$	C-H stretch	A <sub>g</sub>	3050	3040	A <sub>1</sub>	3060	3058
$\nu_2$	C≡N stretch		2215	2212		2240	2232
$\nu_3$	C=C stretch		1610	1603		1600	1600
$\nu_4$	C-H bend i.p		1290	1294		1212	1215
$\nu_5$	C-C stretch		1010	1013		960	963
$\nu_6$	C=C-C bend i.p		596	598		480	480
$\nu_7$	C-C≡N bend i.p		265	266		378	381
$\nu_8$	C-H bend o.p	A <sub>u</sub>	785	782	A <sub>2</sub>	770	768
$\nu_9$	C-C≡N bend o.p		150*	150		275	265
$\nu_{10}$	Torsion		-	121 <sup>c</sup>		112	112
$\nu_{11}$	C-H bend o.p	B <sub>g</sub>	845	845	B <sub>2</sub>	880	880
$\nu_{12}$	C-C≡N bend o.p		*251*	251		*268*	268
$\nu_{13}$	C-H stretch	B <sub>u</sub>	3070	3062	B <sub>1</sub>	3060	3052
$\nu_{14}$	C≡N stretch		2225	2226		2240	2227
$\nu_{15}$	C-H bend i.p		1260	1261		1372	1374
$\nu_{16}$	C-C stretch		1000	1056		1018	1020
$\nu_{17}$	C=C-C bend i.p.		540	543		595	595
$\nu_{18}$	C-C≡N bend i.p		(360)*	363*		*463*	461

i.p. - in-plane, o.p. - out-of-plane, \* frequencies substituted from Ref (9), c- calculated value, + liquid frequencies, ( ) inferred from combination bands

The diagonal elements of the potential energy matrix in Table 4 and Table 5 are the force constants of stretching and bending of bonds. In malononitrile Fujiyama and Shimanouchi [3] have calculated the C≡N and C-C stretching force constants to be 18.2 and 3.2 mdyn/A° respectively. Using Urey-Bradley force field Fujiyama *et al* (11) have calculated the C-C, C-H and C≡N force constants in succinonitrile to be 3.1, 4.2, and 18.3 mdyn/A° respectively. Using the same type of force field, Fujiyama and Shimanouchi have calculated the force constants for malononitrile as  $K_{C-H} = 4.2$ ,  $K_{C-C} = 3.202$ , and  $K_{C≡N} = 18.159$  mdyn/A°. Devlin *et al* have calculated the force constants for acrylonitrile as  $K_{C=C} = 7.51$ ,  $K_{C≡H} = 4.72$ ,  $K_{C≡N} = 17.9$  and  $K_{C-C} = 4.2$  mdyn/A°. The values of the force constant matrix for the respective bonds agree very well with the values of similar bonds in other cyanoethylenes.



Table 4. Symmetrized potential energy matrix for fumaronitrile

Species							
A <sub>g</sub>	S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>4</sub>	S <sub>5</sub>	S <sub>6</sub>	S <sub>7</sub>
S <sub>1</sub>	5.0678	0	0.19375	0.01952	0.04355	-0.00296	-0.00366
S <sub>2</sub>		18 6585	0	0	1 06199	0.10843	-0.03353
S <sub>3</sub>			9 1002	-1.1535	0 76994	-0 39016	0.02058
S <sub>4</sub>				1 1555	-0 25866	0 11864	-0.00376
S <sub>5</sub>		Symm.			3.6338	0.12642	-0 09988
S <sub>6</sub>						1.9642	-0 2242
S <sub>7</sub>							0.31796
Species				Species			
A <sub>u</sub>	S <sub>8</sub>	S <sub>9</sub>	S <sub>10</sub>	B <sub>g</sub>	S <sub>11</sub>	S <sub>12</sub>	
S <sub>8</sub>	1.15292	0 004764	0 003155	S <sub>11</sub>	1 3452	0	
S <sub>9</sub>	Symm.	0.16396	0.00503	S <sub>12</sub>	0	0 45686	
S <sub>10</sub>			0.08851				
Species							
B <sub>u</sub>	S <sub>13</sub>	S <sub>14</sub>	S <sub>15</sub>	S <sub>16</sub>	S <sub>17</sub>	S <sub>18</sub>	
S <sub>13</sub>	5 1415	0	0.06235	0 04048	0 00747	-0 008	
S <sub>14</sub>		18 7955	0	1 45026	0 22722	-0 068633	
S <sub>15</sub>			1 09742	0.019	-0 018639	0 00585	
S <sub>16</sub>		Symm		3.95034	0 61824	-0.20157	
S <sub>17</sub>					1.61441	-0.34124	
S <sub>18</sub>						0 590663	

Table 5. Symmetrized potential energy matrix for malconitrile

Species							
A <sub>1</sub>	S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>4</sub>	S <sub>5</sub>	S <sub>6</sub>	S <sub>7</sub>
S <sub>1</sub>	5.12987	0	0 19281	0.01722	0 04606	-0 00189	-0.00747
S <sub>2</sub>		18 9864	0	0	1 1231	0.06955	-0.06841
S <sub>3</sub>			9 0564	-1.01745	0.81424	-0.25025	0 041996
S <sub>4</sub>				1.01938	-0.27355	0.076103	-0.00768
S <sub>5</sub>		Symm			3.84287	0 08109	-0.20378
S <sub>6</sub>						1 2598	-0.46602
S <sub>7</sub>							0 64868
Species				Species			
A <sub>2</sub>	S <sub>8</sub>	S <sub>9</sub>	S <sub>10</sub>	B <sub>g</sub>	S <sub>11</sub>	S <sub>12</sub>	
S <sub>8</sub>	1.1103	0 0147	0.00274	S <sub>11</sub>	1 4589	0	
S <sub>9</sub>	Symm.	0.50818	0.00435	S <sub>12</sub>	0	0.52084	
S <sub>10</sub>			0.07710				
Species							
B <sub>1</sub>	S <sub>13</sub>	S <sub>14</sub>	S <sub>15</sub>	S <sub>16</sub>	S <sub>17</sub>	S <sub>18</sub>	
S <sub>13</sub>	5.10961	0	0 07404	0.03776	0.00897	-0 012916	
S <sub>14</sub>		18 91121	0	1 35262	0.27285	-0 11077	
S <sub>15</sub>			1.30313	0.017721	-0.02238	0.00944	
S <sub>16</sub>		Symm.		3.6844	0.74242	-0.32534	
S <sub>17</sub>					1.93866	-0.55078	
S <sub>18</sub>						0.95335	

#### 4. Conclusion

A complete vibrational assignment of the fundamentals has been proposed for fumaronitrile and maleonitrile. The force constants for the various bonds for the two molecules calculated through normal coordinate analysis agree well with similar bonds in dicyanoethylenes and other related molecules. The P.E.D. calculated from the force constants have high values thus confirming the assignments of the fundamental frequencies for the two molecules.

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